LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP070323\
Data File : BP015956.D
Acq On : 03 Jul 2023 17:56
Operator : MA/JU
Sample : 03245-14
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DCGH2

Integration Parameters: LSCINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 0.1 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP062623.MA.M
Title : SVOA CALIBRATION

Signal : TIC: BP015956.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.369	27	31	38	rVB	63074	91504	0.66%	0.097%
2	3.816	104	107	112	rVB4	15647	22012	0.16%	0.023%
3	3.863	112	115	120	rVV	21991	40026	0.29%	0.042%
4	3.916	121	124	134	rVV	69037	112053	0.81%	0.119%
5	3.993	135	137	139	rVV3	14133	15561	0.11%	0.017%
6	4.034	139	144	151	rVV	82687	134968	0.98%	0.143%
7	4.093	151	154	158	rVV6	10000	17098	0.12%	0.018%
8	4.140	158	162	167	rVB	20641	31870	0.23%	0.034%
9	5.087	319	323	326	rBV	16734	23657	0.17%	0.025%
10	7.116	662	668	671	rBV8	10198	18881	0.14%	0.020%
11	7.234	679	688	705	rBV	668134	1760621	12.73%	1.869%
12	7.369	705	711	733	rVB	748295	1430393	10.34%	1.519%
13	7.581	740	747	770	rBV	923386	1837695	13.29%	1.951%
14	8.040	818	825	842	rBV	1150717	2224007	16.08%	2.361%
15	8.792	945	953	967	rBV2	673998	1817054	13.14%	1.929%
16	8.904	967	972	989	rVB	136748	318605	2.30%	0.338%
17	9.240	1020	1029	1053	rBV	855072	1847749	13.36%	1.962%
18	9.963	1144	1152	1173	rBV	574756	1539972	11.14%	1.635%
19	10.275	1196	1205	1209	rBV10	13329	34677	0.25%	0.037%
20	10.539	1241	1250	1285	rBV	647004	2171972	15.71%	2.306%
21	10.869	1299	1306	1323	rVV	1690737	3406976	24.64%	3.617%
22	11.057	1330	1338	1362	rBV	351990	1255703	9.08%	1.333%
23	11.863	1471	1475	1480	rVB5	9915	18425	0.13%	0.020%
24	12.498	1577	1583	1590	rVB4	14595	34741	0.25%	0.037%
25	13.045	1669	1676	1677	rBV7	8076	14429	0.10%	0.015%
26	13.075	1677	1681	1687	rVB9	10459	21083	0.15%	0.022%
27	13.204	1698	1703	1706	rBV7	9637	15422	0.11%	0.016%
28	13.286	1714	1717	1725	rVB9	7845	17225	0.12%	0.018%
29	13.492	1748	1752	1757	rBV4	15192	21882	0.16%	0.023%
30	13.575	1757	1766	1773	rVB3	42863	83936	0.61%	0.089%
31	13.757	1788	1797	1802	rBV3	4952	14770	0.11%	0.016%
32	13.880	1813	1818	1823	rBV9	11304	20841	0.15%	0.022%
33	14.004	1832	1839	1845	rBV3	98785	186020	1.35%	0.197%
34	14.110	1849	1857	1871	rBV	1878745	3252077	23.52%	3.453%
35	14.392	1898	1905	1921	rBV2	2519124	4145889	29.98%	4.401%
36	14.557	1929	1933	1941	rVB3	29024	58691	0.42%	0.062%

LSC Area Percent Report

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Sample : 03245-14
Misc :
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Instrument : BNA_P
ClientSampleId : DCGH2

Integration Parameters: LSCINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 0.1 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP062623.MA.M
Title : SVOA CALIBRATION

37	14.627	1941	1945	1950	rBV5	21754	33180	0.24%	0.035%
38	14.698	1950	1957	1972	rBV	2864418	4488924	32.46%	4.766%
39	14.922	1991	1995	1999	rBV7	16096	25468	0.18%	0.027%
40	14.998	2000	2008	2025	rBV2	252701	962164	6.96%	1.021%
41	15.463	2083	2087	2091	rVV7	10207	17721	0.13%	0.019%
42	15.516	2092	2096	2101	rVB2	33090	46818	0.34%	0.050%
43	15.698	2119	2127	2143	rBV	2787046	4935709	35.69%	5.240%
44	15.874	2151	2157	2178	rBV	352691	1000965	7.24%	1.063%
45	16.063	2183	2189	2199	rBV	959040	1501305	10.86%	1.594%
46	16.304	2227	2230	2235	rVB7	17197	25177	0.18%	0.027%
47	16.374	2239	2242	2243	rBV3	28850	28853	0.21%	0.031%
48	16.551	2267	2272	2274	rBV2	29277	43922	0.32%	0.047%
49	16.627	2280	2285	2293	rVB2	66110	110697	0.80%	0.118%
50	16.839	2318	2321	2330	rBV8	16735	32372	0.23%	0.034%
51	16.927	2331	2336	2343	rBV2	73239	127307	0.92%	0.135%
52	17.169	2374	2377	2381	rBV2	41049	58319	0.42%	0.062%
53	17.333	2401	2405	2412	rVB	71221	99292	0.72%	0.105%
54	17.398	2413	2416	2420	rBV6	35266	51719	0.37%	0.055%
55	17.457	2420	2426	2432	rBV	3307599	5046771	36.50%	5.358%
56	17.563	2438	2444	2468	rVB2	2574807	4507990	32.60%	4.786%
57	17.910	2500	2503	2508	rVB2	39952	48847	0.35%	0.052%
58	18.092	2531	2534	2538	rVB6	30909	38557	0.28%	0.041%
59	18.204	2549	2553	2556	rBV5	37343	60417	0.44%	0.064%
60	18.257	2557	2562	2567	rBV	330434	481326	3.48%	0.511%
61	18.316	2567	2572	2580	rBV	2565224	3438279	24.86%	3.650%
62	19.186	2717	2720	2722	rBV	64251	68127	0.49%	0.072%
63	19.398	2753	2756	2757	rBV3	110306	105685	0.76%	0.112%
64	19.421	2757	2760	2762	rVV2	247072	319993	2.31%	0.340%
65	19.463	2765	2767	2775	rVB	461688	609905	4.41%	0.647%
66	19.533	2775	2779	2786	rBV	663788	985052	7.12%	1.046%
67	19.786	2817	2822	2827	rBV	3506313	5310077	38.40%	5.637%
68	20.257	2899	2902	2908	rBV2	252288	370464	2.68%	0.393%
69	20.745	2982	2985	2987	rBV	150784	188891	1.37%	0.201%
70	21.198	3059	3062	3063	rBV2	311192	323023	2.34%	0.343%
71	21.227	3063	3067	3073	rVB	1143569	1667284	12.06%	1.770%
72	21.404	3095	3097	3102	rVB	333135	346017	2.50%	0.367%
73	21.551	3117	3122	3127	rBV	2711020	4053909	29.32%	4.304%
74	23.221	3402	3406	3416	rVB	843053	1431555	10.35%	1.520%
75	23.927	3521	3526	3533	rVB2	1587136	3122571	22.58%	3.315%
76	24.092	3548	3554	3569	rVB	1622604	3941956	28.51%	4.185%

LSC Area Percent Report

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Misc :
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Instrument :
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ClientSampleId :
DCGH2

Integration Parameters: LSCINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 0.1 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
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Title : SVOA CALIBRATION

77	24.650	3644	3649	3657	rVB	1065722	2250835	16.28%	2.390%
78	28.733	4334	4343	4361	rVB3	3621901	13828640	100.00%	14.681%

Sum of corrected areas: 94194568

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Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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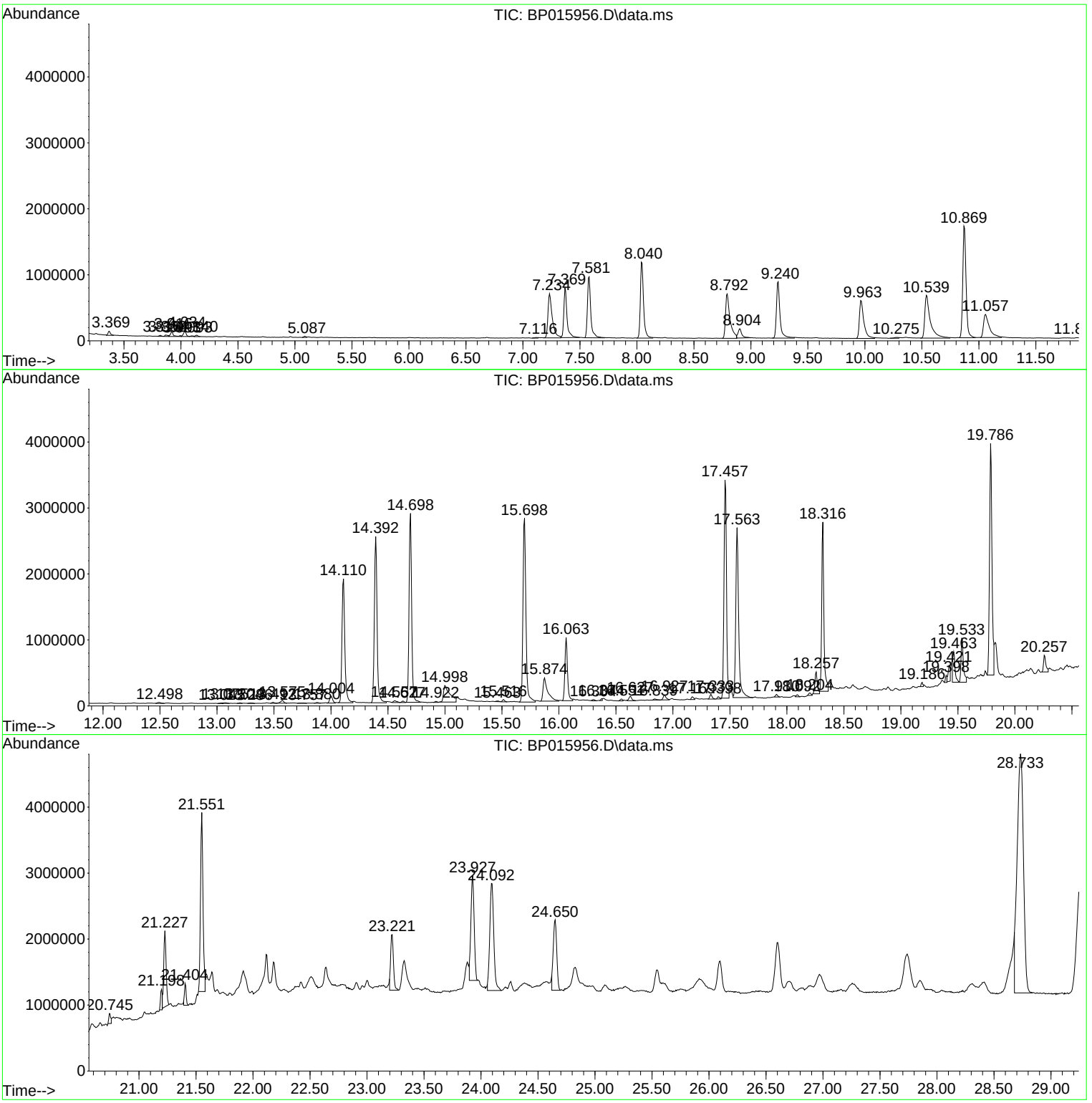
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP062623.MA.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP070323\
Data File : BP015956.D
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Instrument :
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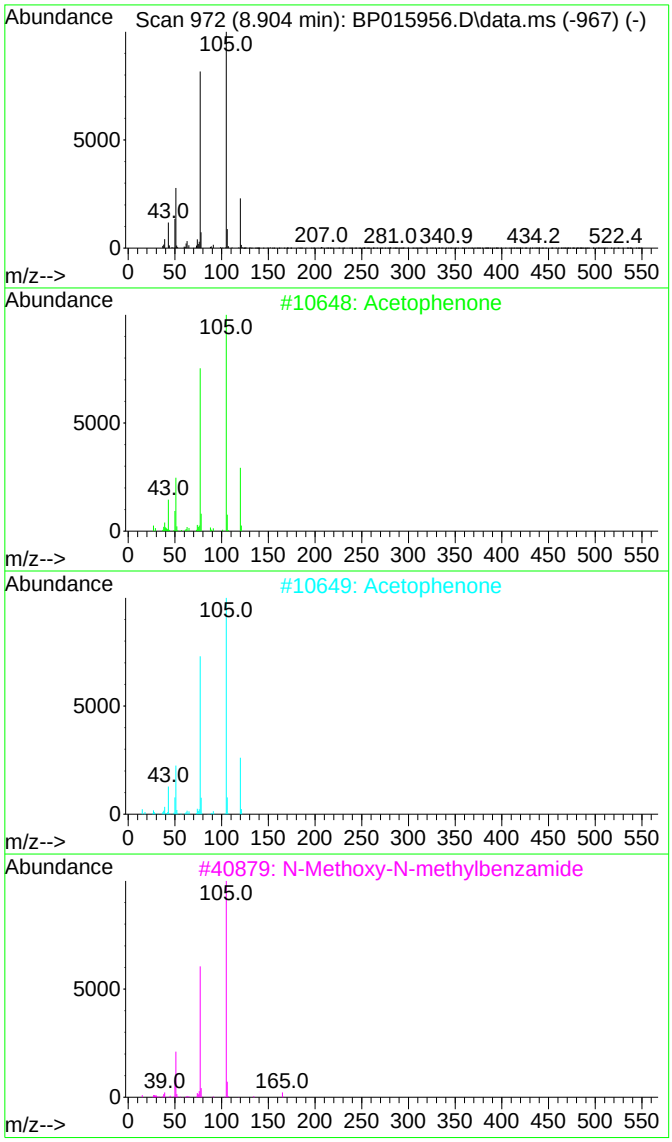
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP062623.MA.M
Quant Title : SVOA CALIBRATION

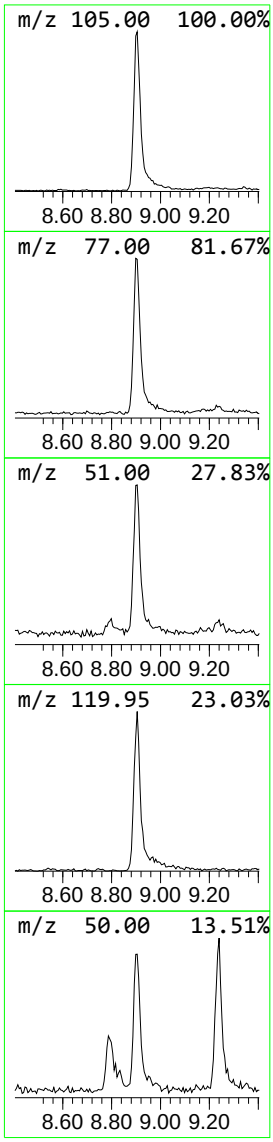
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Aceto phenone Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.904	2.87 ng/ul	318605	1,4-Dichlorobenzene-d4	8.045

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetophenone	120	C8H8O	000098-86-2	91
2	Acetophenone	120	C8H8O	000098-86-2	91
3	N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	72
4	Benzoic acid, 2-propenyl ester	162	C10H10O2	000583-04-0	72
5	Ethanone, 2,2,2-trifluoro-1-phenyl-	174	C8H5F3O	000434-45-7	72





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP070323\
Data File : BP015956.D
Acq On : 03 Jul 2023 17:56
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Sample : 03245-14
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DCGH2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP062623.MA.M
Quant Title : SVOA CALIBRATION

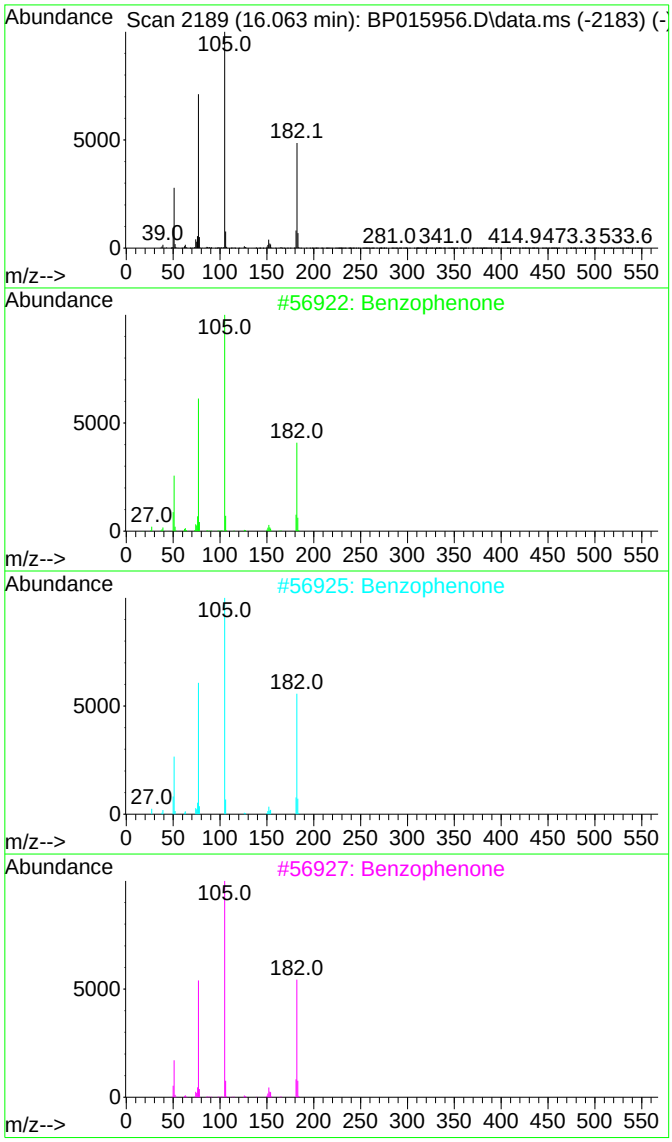
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

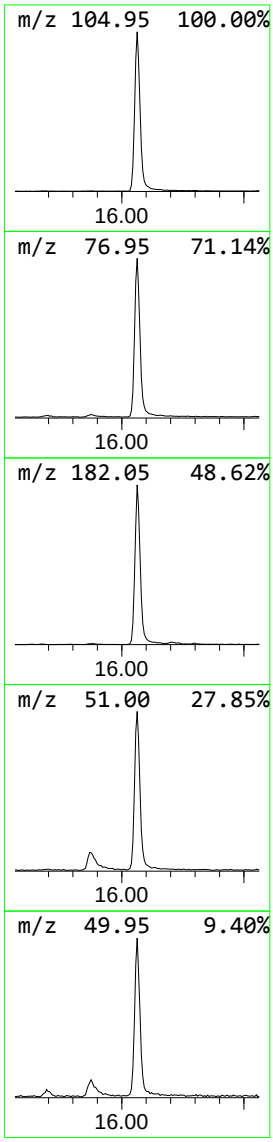
****

Peak Number 2 Benzophenone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.063	6.69 ng/ul	1501310	Acenaphthene-d10	14.698

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Benzophenone	182	C13H10O	000119-61-9	96
3	Benzophenone	182	C13H10O	000119-61-9	95
4	Benzophenone	182	C13H10O	000119-61-9	91
5	Benzophenone	182	C13H10O	000119-61-9	91





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Data File : BP015956.D
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Operator : MA/JU
Sample : 03245-14
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DCGH2

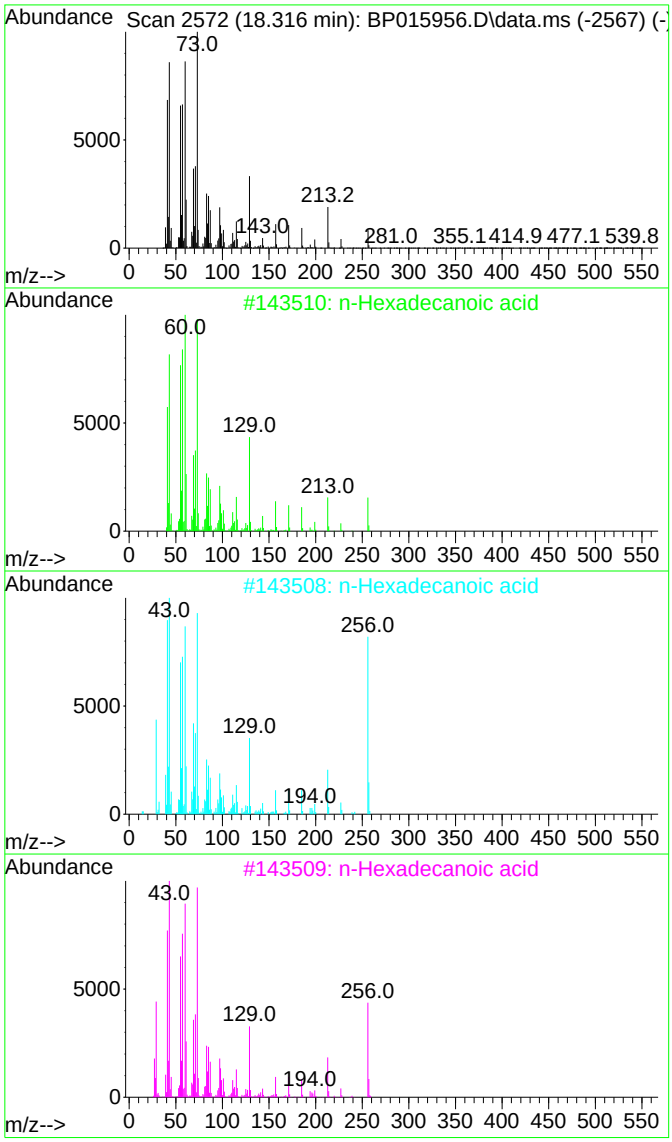
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP062623.MA.M
Quant Title : SVOA CALIBRATION

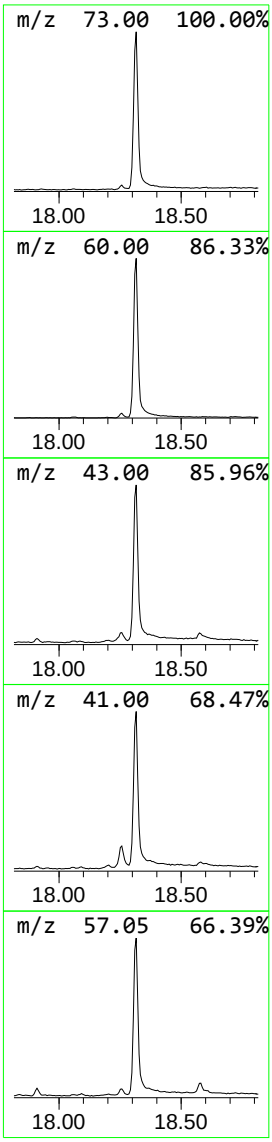
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.316	13.63 ng/ul	3438280	Phenanthrene-d10	17.457

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	95





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ALS Vial : 10 Sample Multiplier: 1

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP062623.MA.M
Quant Title : SVOA CALIBRATION

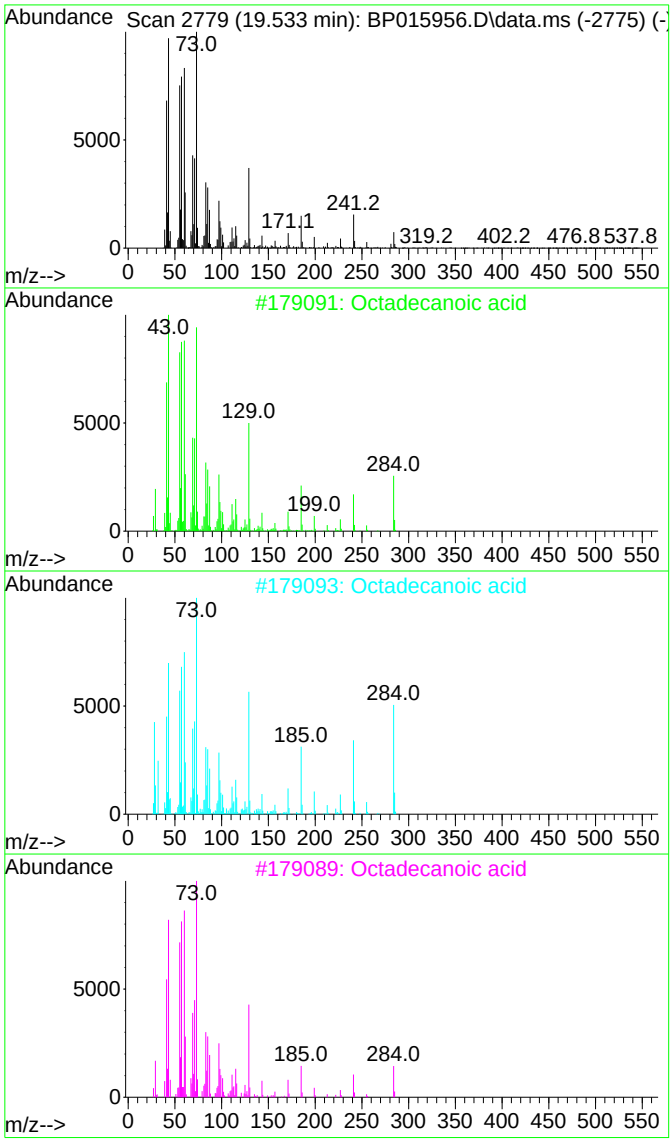
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

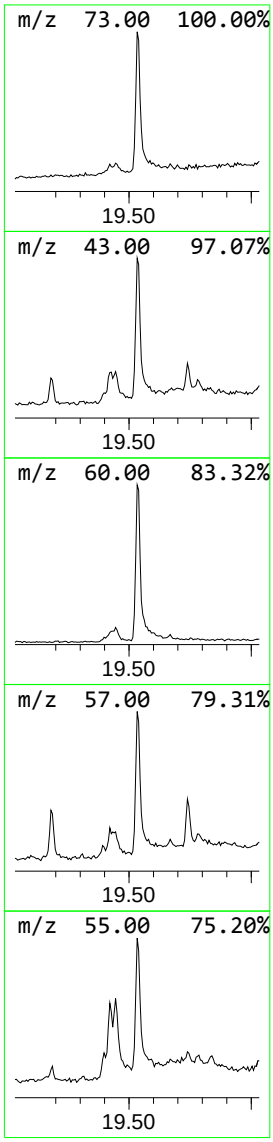
****

Peak Number 4 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.533	4.86 ng/ul	985052	Chrysene-d12	21.551

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Octadecanoic acid	284	C18H36O2	000057-11-4	99
3	Octadecanoic acid	284	C18H36O2	000057-11-4	97
4	Octadecanoic acid	284	C18H36O2	000057-11-4	95
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	93





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ALS Vial : 10 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP062623.MA.M
Quant Title : SVOA CALIBRATION

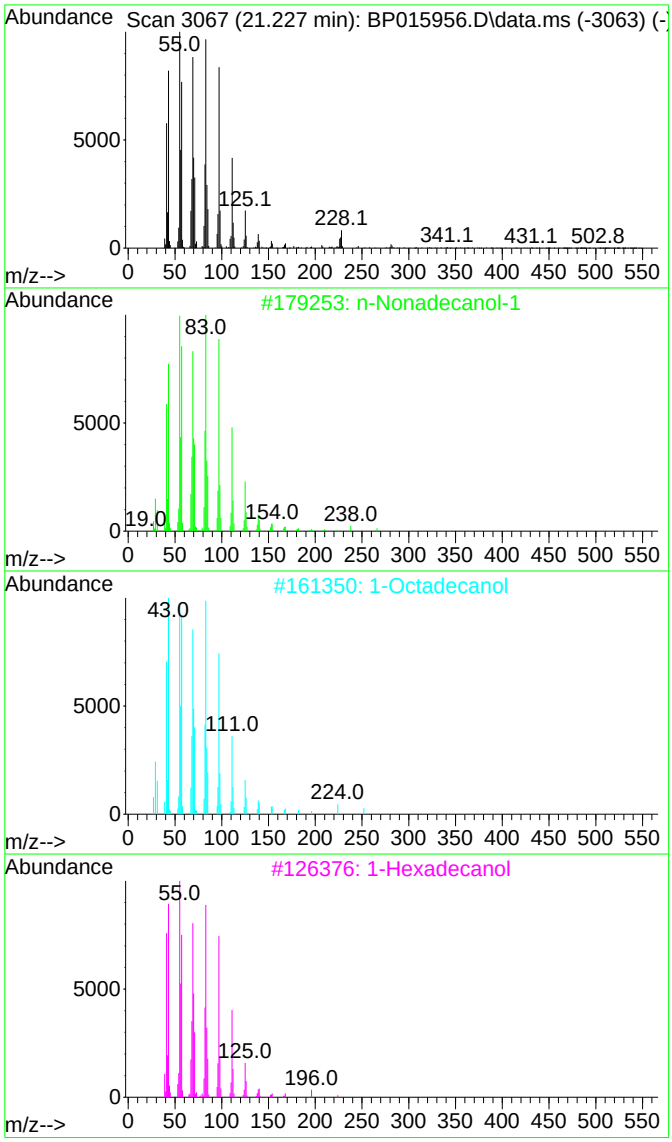
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

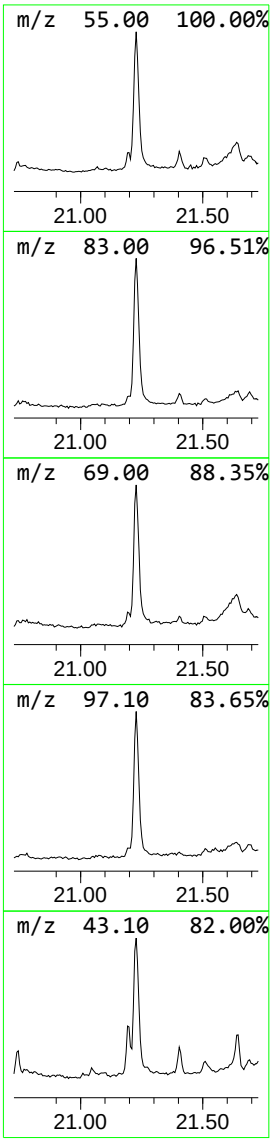
****

Peak Number 5 n-Nonadecanol-1 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.227	8.23 ng/ul	1667280	Chrysene-d12	21.551

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Nonadecanol-1	284	C19H40O	001454-84-8	94
2	1-Octadecanol	270	C18H38O	000112-92-5	94
3	1-Hexadecanol	242	C16H34O	036653-82-4	93
4	1-Hexadecanol	242	C16H34O	036653-82-4	91
5	Cyclohexadecane	224	C16H32	000295-65-8	91





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ALS Vial : 10 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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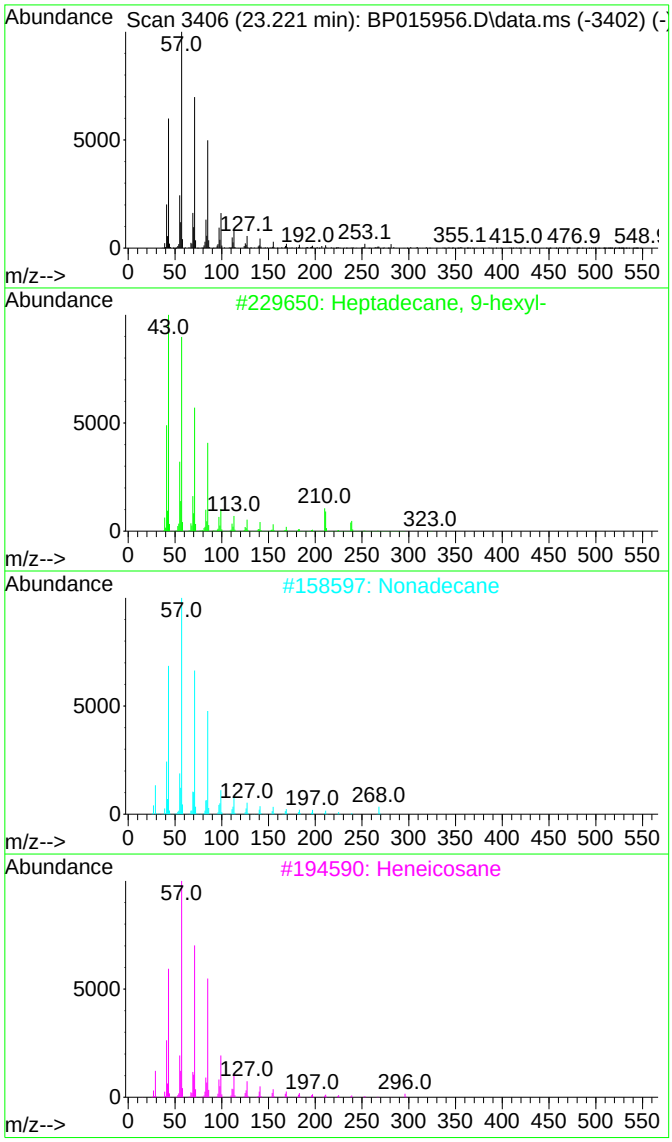
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP062623.MA.M
Quant Title : SVOA CALIBRATION

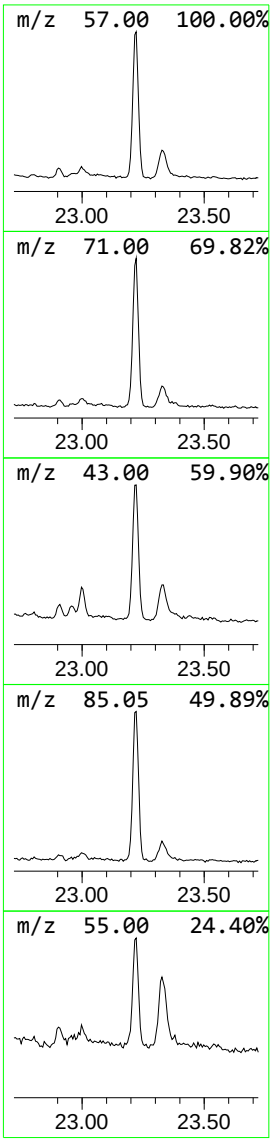
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 (DEL) Alkane: Straight-Chai... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.221	7.26 ng/ul	1431560	Perylene-d12	24.098

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 9-hexyl-	324	C23H48	055124-79-3	94
2	Nonadecane	268	C19H40	000629-92-5	93
3	Heneicosane	296	C21H44	000629-94-7	91
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
5	Tetracosane	338	C24H50	000646-31-1	91





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Sample : 03245-14
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DCGH2

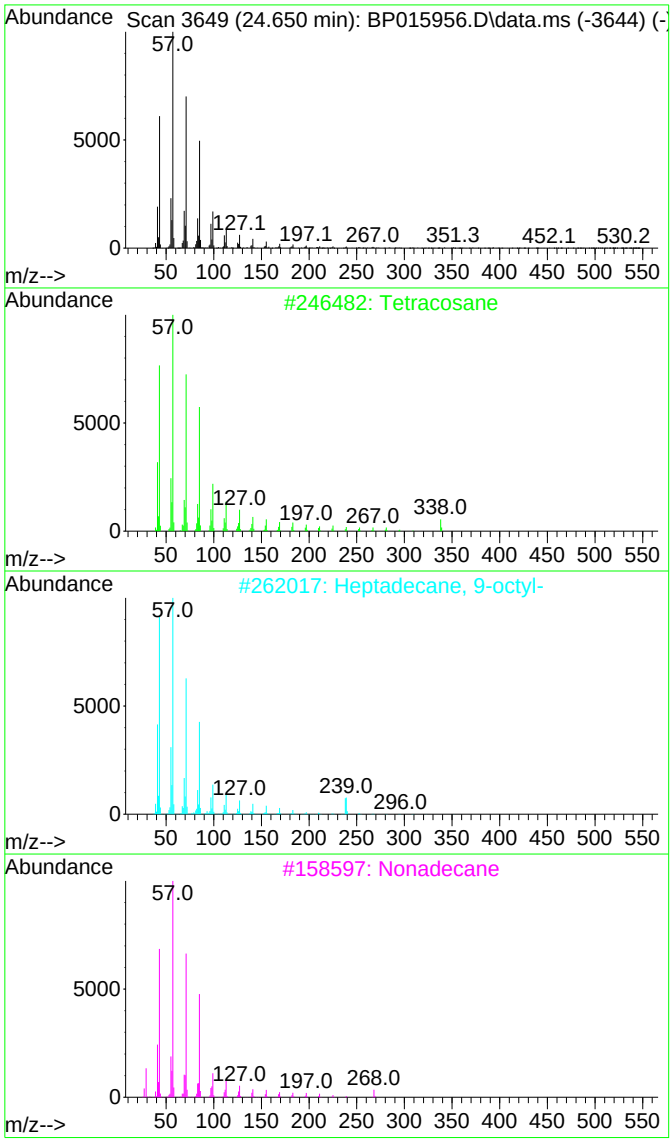
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP062623.MA.M
Quant Title : SVOA CALIBRATION

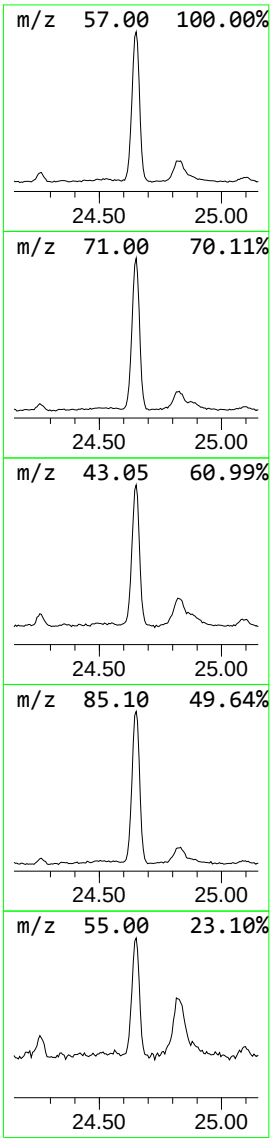
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 (DEL) Alkane: Straight-Chai... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.651	11.42 ng/ul	2250840	Perylene-d12	24.098

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	97
2	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	95
3	Nonadecane	268	C19H40	000629-92-5	93
4	2-Methyltetracosane	352	C25H52	001560-78-7	93
5	Pentacosane	352	C25H52	000629-99-2	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP070323\
Data File : BP015956.D
Acq On : 03 Jul 2023 17:56
Operator : MA/JU
Sample : 03245-14
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DCGH2

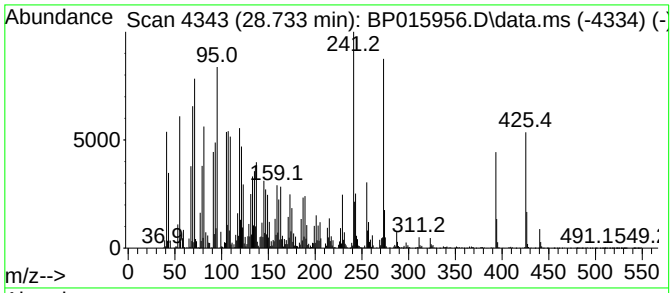
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP062623.MA.M
Quant Title : SVOA CALIBRATION

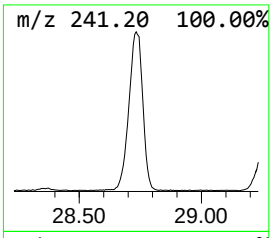
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

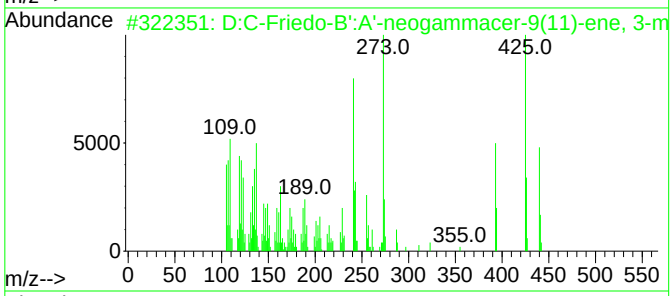
****
Peak Number 8 D:C-Friedo-B':A'-neogammace... Concentration Rank 1

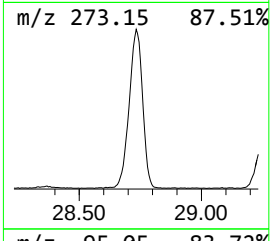
R.T.	EstConc	Area	Relative to ISTD	R.T.
28.733	70.16 ng/ul	13828600	Perylene-d12	24.098

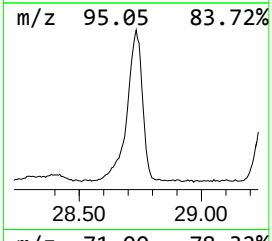
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	D:C-Friedo-B':A'-neogammacer-9(1...	440	C31H52O	004555-56-0	59
2	Undec-10-ynoic acid, 2,7-dimethy...	316	C21H32O2	1000406-96-7	27
3	(.+/-.)-Lavandulol, pentafluorop...	300	C13H17F5O2	1000352-63-1	25
4	.beta.-Alanine, N-(2-furoyl)-, p...	393	C23H39NO4	1000321-98-4	25
5	Lupeol	426	C30H50O	000545-47-1	22

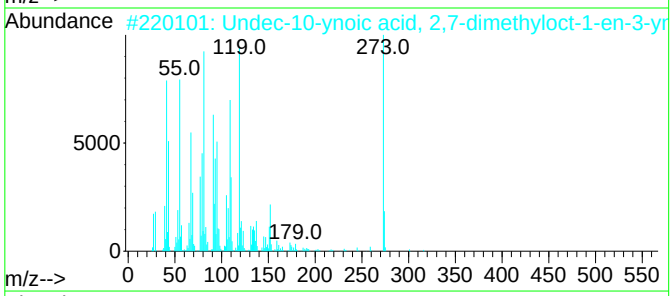


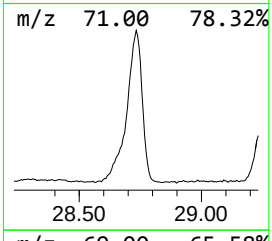


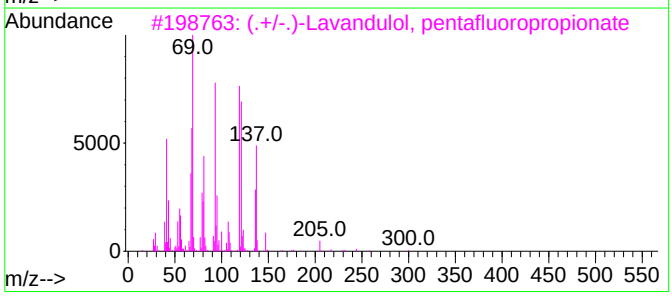


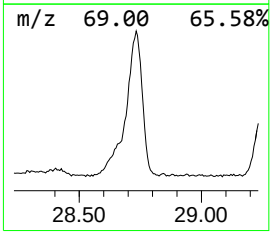












Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP070323\
Data File : BP015956.D
Acq On : 03 Jul 2023 17:56
Operator : MA/JU
Sample : 03245-14
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Aceto phenone	8.904	2.9	ng/ul	318605	1	8.045	2224010	20.0
Benzophenone	16.063	6.7	ng/ul	1501310	3	14.698	4488920	20.0
n-Hexadecanoic ...	18.316	13.6	ng/ul	3438280	4	17.457	5046770	20.0
Octadecanoic acid	19.533	4.9	ng/ul	985052	5	21.551	4053910	20.0
n-Nonadecanol-1	21.227	8.2	ng/ul	1667280	5	21.551	4053910	20.0
(DEL) Alkane: S...	23.221	7.3	ng/ul	1431560	6	24.098	3941960	20.0
(DEL) Alkane: S...	24.651	11.4	ng/ul	2250840	6	24.098	3941960	20.0
D:C-Friedo-B':A...	28.733	70.2	ng/ul	13828600	6	24.098	3941960	20.0